Rock Salt/Halite (NaCl, $B1$) Structure: AB_cF8_225_a_b-001

This structure previously used the label(s) `AB_cF8_225_a_b`. Calls to these addresses will be redirected here.

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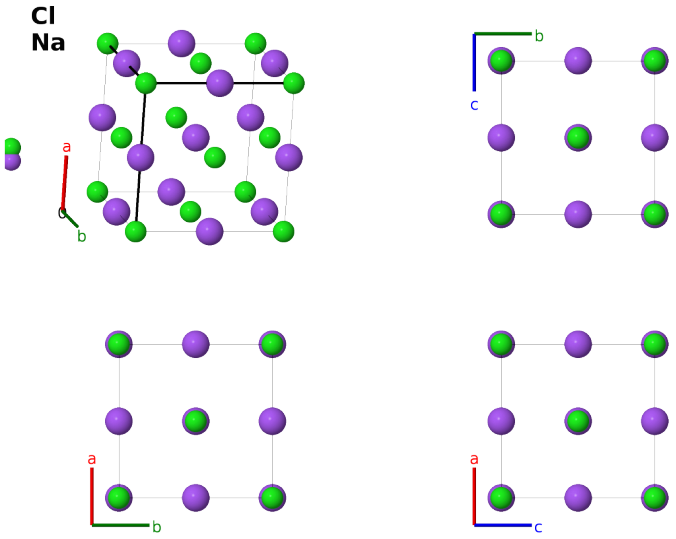
https://aflow.org/prototype-encyclopedia/Q53X

https://aflow.org/prototype-encyclopedia/AB_cF8_225_a_b-001



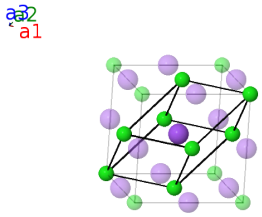
Prototype	ClNa
AFLOW prototype label	AB_cF8_225_a_b-001
***Strukturbericht* designation**	$B1$
Mineral name	halite
ICSD	240598
CCDC	1711262
Pearson symbol	cF8
Space group number	225
Space group symbol	$Fm\bar{3}m$
AFLOW prototype command	`aflow --proto=AB_cF8_225_a_b-001 --params=`a

Other compounds with this structure

AgCl, AmO, BaO, BaPo, BaS, BaSe, BaTe, CaO, CaPo, CaS, CaSe, CdO, CeAs, CeBi, CeN, CeP, CeS, CeSb, CeSe, CeTe, CoO, CrN, DyAs, DyBi, DyN, DyP, DyS, DySb, DySe, DyTe, ErAs, ErBi, ErN, ErP, ErS, ErSb, ErSe, ErTe, EuN, EuO, EuS, EuSe, EuTe, GdAs, GdN, GdSb, GdSe, GdTe, HfB, HfC, HfN, HoAs, HoBi, HoN, HoP, HoS, HoSb, HoSe, HoTe, KBr, LaAs, LaBi, LaN, LaP, LaS, LaSb, LaTe, LiCl, LiF, LiH, LuN, LuS, LuSb, MgO, MgS, MgSe, MnO, MnS, MnSe, MnTe, NU, NaBr, NaF, NaH, NbO, NdAs, NdBi, NdN, NdP, NdS, NdTe, NiO, NpC, NpN, NpO, PaO, PbPo, PbS, PbSe, PbTe, PdH, PrAs, PrBi, PrN, PrP, PrS, PrSb, PrSe, PuAs, PuB, PuBi, PuC, PuN, PuO, PuP, PuS, PuTe, RbF, RbH, ScAs, ScBi, ScC, ScN, ScP, ScSb, SmAs, SmN, SmO, SmP, SmS, SmSe, SmTe, SmTm, SnAs, SnSb, SnSe, SrO, SrS, SrTe, TaC, TaO, TbAs, TbBi, TbN, TbP, TbS, TbSb, TbSe, TbTe, ThAs, ThC, ThGe, ThN, ThSb, TiC, TiN, TiO, TmAs, TmBi, TmN, TmP, TmSb, TmSe, TmTe, UAs, UBi, UC, UO, UP, US, USb, USe, UTe, VO, YAs, YBi, YN, YP, YS, YSb, YSe, YTe, YbAs, YbN, YbO, YbP, YbS, YbSb, YbSe, YbTe, ZnSe, ZrB, ZrC, ZrN, ZrO, ZrS

Face-centered Cubic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Cl I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(4b)	Na I

References

[1] D. Walker, P. K. Verma, L. M. D. Cranswick, R. L. Jones, S. M. Clark, and S. Buhre, *Halite-sylvite thermoelasticity*, Am. Mineral. **89**, 204–210 (2004).

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

First cited in

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